

NEURAL NETWORK AND METHOD OF TRAINING

DESCRIPTION

FIELD OF THE INVENTION

[Para 1] The present invention relates to neural networks.

DESCRIPTION OF RELATED ART

[Para 2] The proliferation of computers accompanied by exponential increases in their processing power has had a significant impact on society in the last thirty years.

[Para 3] Commercially available computers are, with few exceptions, of the Von Neumann type. Von Neumann type computers include a memory and a processor. In operation, instructions and data are read from the memory and executed by the processor. Von Neumann type computers are suitable for performing tasks that can be expressed in terms of sequences of logical or arithmetic steps. Generally, Von Neumann type computers are serial in nature; however, if a function to be performed can be expressed in the form of a parallel algorithm, a Von Neumann type computer that includes a number of processors working cooperatively in parallel can be utilized.

[Para 4] For certain classes of problems, algorithmic approaches suitable for implementation on a Von Neumann machine have not been developed. For other classes of problems, although algorithmic approaches to the solution have been conceived, it is expected that executing the conceived algorithm would take an unacceptably long period of time.

[Para 5] Inspired by information gleaned from the field of neurophysiology, alternative means of computing and otherwise processing information known as neural networks were developed. Neural networks generally include one or more inputs, and one or more outputs, and one or more processing nodes intervening between the inputs and outputs. The foregoing are coupled by

signal paths (directed edges) characterized by weights. Neural networks that include a plurality of inputs and that are aptly described as parallel due to the fact that they operate simultaneously on information received at the plurality of inputs have also been developed. Neural networks hold the promise of being able handle tasks that are characterized by a high input data bandwidth. In as much as the operations performed by each processing node are relatively simple and are predetermined, there is the potential to develop very high speed processing nodes and from them high speed and high input data bandwidth neural networks.

[Para 6] There is generally no overarching theory of neural networks that can be applied to design neural networks to perform a particular task. Designing a neural network involves specifying the number and arrangement of nodes, and the weights that characterize the interconnection between nodes. A variety of stochastic methods have been used in order to explore the space of parameters that characterize a neural network design in order to find suitable choices of parameters, that lead to satisfactory performance of the neural network. For example, genetic algorithms and simulated annealing have been applied to the design neural networks. The success of such techniques is varied, and they are also computationally intensive.

BRIEF DESCRIPTION OF THE FIGURES

[Para 7] The present invention will be described by way of exemplary embodiments, but not limitations, illustrated in the accompanying drawings in which like references denote similar elements, and in which:

[Para 8] FIG. 1 is a graph representation of a neural network according to a first embodiment of the invention;

[Para 9] FIG. 2 is a block diagram of a processing node used in the neural network shown in FIG. 1;

[Para 10] FIG. 3 is a table of weights that characterize directed edges from inputs to processing nodes and between processing nodes in a hypothetical neural network of the type shown in FIG. 1;

[Para 11] FIG. 4 is a table of weights showing how a topology of the type shown in FIG. 1 can be transformed into a three-layer perceptron by zeroing selected weights;

[Para 12] FIG. 5 is a table of weights showing how a topology of the type shown in FIG. 1 can be transformed into a multi-output, multi-layer perceptron by zeroing selected weights;

[Para 13] FIG. 6 is a graph representing the topology reflected in FIG. 5;

[Para 14] FIG. 7 is a flow chart of a method of training the neural networks of the types shown in FIGs. 1,6 according to the preferred embodiment of the invention;

[Para 15] FIG. 8 shows several subgraphs illustrating that the number of signal paths between two nodes is dependent on the number nodes which separate the two nodes;

[Para 16] FIG. 9 shows several subgraphs illustrating particular signal paths between two nodes that are considered in evaluating a linear approximation of the derivative of an output from a network with respect to a particular weight;

[Para 17] FIG. 10 is a table of randomly generated weights describing a network of the type shown in FIG. 10, that is used to evaluate the accuracy of linear estimates of derivatives of an output with respect to particular weights;

[Para 18] FIG. 11 is a table of derivatives calculated using the randomly generated weights shown in FIG. 10;

[Para 19] FIG. 12 is a table of highly accurate, low computation cost estimates of the derivatives shown in FIG. 11;

[Para 20] FIG. 13 is a flow chart of a method of selecting the number of nodes in neural networks of the types shown in FIGs. 1, 6 according to the preferred embodiment of the invention; and

[Para 21] FIG. 14 is a block diagram of a computer used to execute the algorithms shown in FIGs. 7, 13 according to the preferred embodiment of the invention.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENTS

[Para 22] As required, detailed embodiments of the present invention are disclosed herein; however, it is to be understood that the disclosed embodiments are merely exemplary of the invention, which can be embodied in various forms. Therefore, specific structural and functional details disclosed herein are not to be interpreted as limiting, but merely as a basis for the claims and as a representative basis for teaching one skilled in the art to variously employ the present invention in virtually any appropriately detailed structure. Further, the terms and phrases used herein are not intended to be limiting; but rather, to provide an understandable description of the invention.

[Para 23] FIG. 1 is a graph representation of a feed forward neural network 100 according to a first embodiment of the invention. The neural network 100 includes a first input 102, a second input 104, a third input 106 and a fourth input 108. The inputs 102–108 can be referred to as input nodes. A fixed bias signal, e.g., input value 1.0, is applied to the first input 102. The neural network 100 further comprises a first processing node 110, a second processing node 112, a third processing node 114, and a fourth processing node 116. The fourth processing node 116 includes an output 118 that serves as a first output of the output of the neural network. A second output 128 of the neural network 100 is tapped from an output of the third processing node 114. The first two processing nodes 110, 112 are hidden nodes in as much as they do not directly supply output externally. Initially, at the outset of training at least, each of the inputs 102, 104, 106, 108 is preferably considered to be coupled by directed edges (e.g., 120, 122) to each of the processing nodes 110, 112, 114, 116. Also, initially at least, every processing node except the last 116 is preferably considered to be coupled by directed edges (e.g. 124, 126) to processing nodes that are downstream (closer to the fourth processing

node 116). The direction of the directed edges is such that signals always pass from lower numbered processing nodes to higher numbered processing nodes (e.g., from the first processing node 110, to the third processing node 114). For a feed forward neural network of the type shown in FIG. 1 that has n inputs, and m processing nodes there are up to:

EQU. 1

$$K = (n + 1)m + \frac{1}{2}m(m - 1)$$

directed edges each of which is characterized by a weight.

[Para 24] In Equation One, n+1 is the number of signal inputs, and m is the number of processing nodes. Note that n is the number of signal inputs other than the fixed bias signal input 102.

[Para 25] A characteristic of the feed forward network topology illustrated in FIG. 1 is that a signal can be coupled from one of a pair of nodes to a second of the pair of nodes, and both of the same pair of nodes can receive signals from a third node. For example, with reference to FIG. 1 the first processing node 110, is coupled to the second 112 and third 114 processing nodes by directed edges, and the second 112 and third 114 processing nodes are also coupled by a directed edge. This characteristic distinguishes the generalized neural network illustrated in FIG. 1, from a perceptron in which nodes are arranged in layers and do not receive signals from other nodes in the same layers. Note, however that a perceptron is a special case of the generalized neural network that can be obtained by selectively eliminating certain directed edges.

[Para 26] Neural networks of the type shown in FIG. 1 can for example be used in control applications where the inputs 104, 106, 108 are coupled to a plurality of sensors, and the outputs 118, 128 are coupled to output transducers.

[Para 27] In an electrical hardware implementation of the invention, the directed edges (e.g., 120, 122) are suitably embodied as attenuating and/or

amplifying circuits. The processing nodes 110, 112, 114, 116 receive the bias signal and input signals from the four inputs 102–108. The bias signal and the input signals are multiplied by weights associated with directed edges through which they are coupled.

[Para 28] The neural network 100 is trained to perform a desired function. Training is akin to programming a Von Neumann computer in that training adapts the neural network 100 to perform a desired function. In as much as signal processing that is performed by the processing nodes 110–116 is preferably unaltered in the course of training the neural network 100 training is achieved by properly selecting the weights that are associated with the plurality of directed edges of the neural network. Training is discussed in detail below with reference to FIG. 7.

[Para 29] FIG. 2 is a block diagram of the first processing node 110 of the neural network 100 shown in FIG. 1. The first processing node 110 includes four inputs 202 that serve as inputs of a summer 204. In the case of the first processing node the inputs 202 receive signals directly from the inputs 102, 104, 106, 108 of the neural network 100. The summer 204 outputs a sum signal to transfer function block 206. The transfer function block 206 applies a transfer function to the sum signal and outputs a result as the processing node's output at an output 208. The transfer function is preferably the sigmoid function:

EQU. 2

$$h_j = \frac{1}{1 + e^{-H_j}}$$

where, h_j is the output of the transfer function block 206, and the output of a j th processing node e.g., processing node 110; and H_j is the summed input of a j th processing node e.g., the output of the summer 204.

[Para 30] The output 208 is coupled through a plurality of directed edges to the second 112, third 114, and fourth 116 processing nodes.

[Para 31] For classification problems, the expected output of the neural network 100 is chosen from a finite set of values e.g., one or zero, which respectively specify that a given set of inputs does or does not belong to a certain class. In classification problems, it is appropriate to use signals that are output by a threshold type (e.g., sigmoid) transfer function at the processing nodes that are used as outputs. The sigmoid function is aptly described as a threshold function in that it rapidly swings from a value near zero to a value near 1 near the domain value of zero. On the other hand, for regression type problems it is preferred to take the output at processing nodes that serve as outputs of a neural network of the type shown in FIG. 1 from the output of summers within those output processing nodes, and not process the final output signals by the sigmoid functions in the output processing nodes. This is appropriate because for regression problems the output is generally expected to be continuous as opposed to consisting of a finite set of discrete values.

[Para 32] Alternatively, in lieu of the sigmoid function other functions or approximations of the sigmoid or other functions are used as the transfer function that is performed by the transfer function block 206. For example, the Gaussian function is alternatively used in lieu of the sigmoid function.

[Para 33] The other processing nodes 112, 114, 116 preferably have the same design as shown in FIG. 2, with the exception that the other processing nodes include summers with different numbers of inputs in order to accommodate input signals from the neural network inputs 102–108 and from other processing nodes. In a hardware implementation of the neural network, the first processing nodes and other processing nodes are implemented in digital or analog circuitry or a combination thereof.

[Para 34] As will be discussed below, in the interest of providing less complex neural networks, according to embodiments of the invention some of the possible directed edges (as counted by Equation One) are eliminated. A method of selecting which directed edges to eliminate in order to provide a less complex and costly neural network is described below with reference to FIG. 7.

[Para 35] FIG. 3 is a table 300 of weights that characterize directed edges from inputs to processing nodes and between processing nodes in a hypothetical neural network of the type shown in FIG. 1. The first column of the table 300 identifies inputs of processing nodes. The subscripted capital H's appearing in the first column stand for the output of the summer in a processing node identified by the subscript.

[Para 36] The left side of the first row of table 300 (to the left of line 302) identifies inputs of the neural network. The left side of the first row includes subscripted X's where the subscript identifies a particular input. For example in the case of the neural network shown in FIG. 1 the neural network inputs 102, 104, 106, 108 would be identified in the left side of the first row as X_0 , X_1 , X_2 , and X_3 . The first input identified by X_0 is the input for the fixed bias (e.g., 102, in neural network 100). The entries in the left hand side of the table 300 which appear as double subscripted capital W's represent weights that characterize directed edges that couple the neural network's inputs to the neural network's processing nodes. The first subscript of each of the capital W's identifies a processing node at which a directed edge characterized by the weight symbolized by the subscripted W terminates, and the second subscript identifies a neural network input at which the directed edge characterized by the weight symbolized by the subscripted W originates.

[Para 37] The right side of the first row identifies outputs of each, except for the last, processing node by a subscripted lower case h. The subscript of on each lower case h identifies a particular processing node. The entries in the right side of the table 300 are double-subscripted capital V's. The subscripted capital V's represent weights that characterize directed edges that couple processing nodes of the neural network. The first subscript of each V identifies a processing node at which the directed edge that is characterized by the weight symbolized by the V in question terminates, whereas the second subscript identifies a processing node at which the directed edge characterized by the weight symbolized by the V in question originates.

[Para 38] All the weights in each row have the same first subscript, which is equal to the subscript of the capital H in the same row of the first column of

the table, which identifies a processing node at which the directed edges characterized by the weights in the row terminate. Similarly, weights in each column of the table have the same second index that identifies an input (on the left hand side of the table 300) or a processing node (on the right hand side of the table) at which the directed edges characterized by the weights in each column originate. Note that the right side of table 300 has a lower triangular form. The latter aspect reflects the feed forward only character of neural networks according to embodiments of the invention.

[Para 39] Table 300 thus concisely summarizes important information that characterizes a neural network.

[Para 40] FIG. 4 is a table 400 of weights showing how a topology of the type shown in FIG. 1 can be transformed into a three-layer perceptron by zeroing out selected weights. As reflected on the left hand side (to the left of heavy line 402) a plurality of processing nodes up to an $(m-1)$ th processing node (shown explicitly for the first three processing nodes) are coupled to a number n of neural network inputs. The first neural network input labeled X_0 serves as a fixed bias signal input. As reflected on the right hand side of the table 400 there is no inter-coupling between the processing nodes (1^{st} to $(m-1)$ th) that are coupled to the inputs. This is represented by zero entries for the weights that characterize directed edges between those processing nodes. The first $m-1$ processing nodes effectively serve as a hidden layer of a single hidden layer perceptron. As indicated by entries in the right side of the last row of the table, the processing nodes m to $m-1$ that are directly coupled to the signal inputs X_1 to X_n are coupled to an m th processing node that serves as an output of the neural network. Thus by eliminating certain directed edges of a feed forward network of the type shown in FIG. 1, such a feed forward network can be transformed into a perceptron having a plurality of processing nodes organized in a single hidden layer. Additional output processing nodes that are coupled to the first $m-1$ processing nodes can also be added to obtain a plural output single hidden layer perceptron.

[Para 41] FIG. 5 is a table 500 of weights showing how a topology of the type shown in FIG. 1 can be transformed into a multi-output, multi- hidden-layer

perceptron by zeroing out selected weights and FIG. 6 is a graph of a neural network 600 representing the topology reflected in FIG. 5. The table 500 reflects that the neural network 600 has n inputs labeled X_0 to X_n . The first input denoted X_0 is preferably used as a fixed bias signal input. (Note that the same X_0 appears in several places in FIG. 6) The neural network 600 further comprises m processing nodes labeled 1 to m . The column for the first, fixed bias signal input X_0 includes weights that act as scaling factors for the biases applied to the m processing nodes. A first block section 502 of the table 500 reflects that the signal inputs $X_1 - X_N$ are coupled to the first $k-1$ processing nodes. A second block section 504 reflects that the signal inputs $X_1 - X_N$ are not coupled to the remaining $m-k+1$ processing nodes of the neural network 600.

[Para 42] A third block section 506 reflects that outputs of the first $k-1$ processing nodes (that are coupled to the inputs $X_1 - X_N$) are coupled to inputs of next $s-k+1$ processing nodes that are labeled by subscripts ranging from k to s . Zeros above the third block 506 indicate that in this example there is no intercoupling among the first $k-1$ processing nodes, and that the neural network is a feed forward network. Zeros below the third block 506 indicate that no additional processing nodes receive signals from the first $k-1$ processing nodes.

[Para 43] Similarly, a fourth block 508 reflects that a successive set of $t-s$ processing nodes labeled $s+1$ to t receives signals from processing nodes labeled k to s . Zeros above the fourth block 508 reflect the feed forward nature of the neural network 600, and that there is no inter-coupling between the processing nodes labeled k to s . The zeros below the fourth block 508 reflect that no further processing nodes beyond those labeled $s+1$ to t receive signals from the processing nodes labeled k to s .

[Para 44] A fifth block 510 reflects that a set of processing nodes labeled $m-2$ to m , that serve as outputs of the neural network 600 described by the table 500, receive signals from processing nodes labeled $s+1$ to t . Zeros above the fifth processing block 510 reflect the feed forward nature of the network 600,

and that no processing nodes other than those labeled $m-2$ to m receive signals from processing nodes labeled $s+1$ to t .

[Para 45] Thus, the table 500 illustrates that by selectively eliminating directed edges (tantamount to zeroing associated weights) a neural network of the type illustrated in FIG. 1, but having a greater number of processing nodes, can be transformed into the multi-input, multiple hidden layer perceptron shown in FIG. 6. In the case illustrated in FIGs. 5-6, processing nodes 1 to $k-1$ serve as a first hidden layer, processing nodes k to s serve as a second hidden layer, and nodes $s+1$ to t serve as a third hidden layer.

[Para 46] In neural networks of the type shown in FIG. 1, the summed input H_k to a k th processing node is given by:

EQU. 3

$$H_k = \sum_{i=0}^n W_{ki} X_i + \sum_{j=1}^{k-1} V_{kj} h_j$$

where, X_i is an i th input that is coupled to the k th processing node;
 W_{ki} is a weight that characterizes a directed edge from the i th input to the k th processing node;
 h_j is the output of a j th processing node that is coupled to the k th processing node; and
 V_{kj} is a weight that characterizes a directed edge from the j th processing node to the k th processing node.

[Para 47] The output of the k th processing node is then given by Equation Two. Thus by repeated application of Equations Two and Three a specified input vector $[X_0...X_n]$ can be propagated through a neural network of the type shown in FIG. 1 (and variations thereof obtained by selectively zeroing weights) and the output of such a neural network at one or more output processing nodes can be calculated.

[Para 48] FIG. 7 is a flow chart of a method 700 of training neural networks of the general type shown in FIG. 1 according to the preferred embodiment of the

invention. Although the method 700 is preferably performed using a computer model of a neural network, the results found using the method, can then be applied to a hardware implemented neural network.

[Para 49] Referring to FIG. 7, in block 702 weights that characterize directed edges of the neural network to be trained are initialized. The weights can for example be initialized randomly, initialized to some predetermined number (e.g., one), or initialized to some values entered by the user (e.g., based on experience or guesses).

[Para 50] Block 704 is the start of a loop that uses successive sets of training data. The training data preferably includes a plurality of sets of training data that represent the domain of input that the neural network to be trained is expected to process. Each k th training data set preferably includes a vector of inputs $X_k=[X_0...X_n]_k$ and an associated expected output Y_k or a vector of expected outputs $Y_k=[Y_{m-q}...Y_m]_k$ in the case of a multi-output neural network.

[Para 51] In block 706 the input vector of the a k th set of training data is applied to the neural network being trained, and in block 708 the input vector of the k th set of training data is propagated through the neural network. Equations Two and Three are used to propagate the training data input through the neural network being trained. In executing block 708 the output of each processing node is determined and stored, at least temporarily, so that such output can be used later in calculating derivatives as described below.

[Para 52] In step 710 the difference between the output of the neural network produced by the k th vector of training data inputs, and the associated expected output for the k th training data is computed. In the case of single output neural network regression the difference is given by:

EQU. 4

$$\Delta R_k = H_m(W, V, X_k) - Y_k$$

[Para 53] where ΔR_k is the difference between the output produced in response the k th training data input vector X_k , and the expected output Y_k that

is associated with the input vector X_k ; $H_m(W,V,X_k)$ is the output (at an m th processing node) of the neural network produced in response to the k th training data input vector X_k . The bold face W represent the set of weights that characterize directed edges from the neural network inputs to the processing nodes; and the bold face V represents the set of weight that characterized directed edges that couple processing nodes. H_m is a function of W , V and X_k . As mentioned above for regression problems a threshold transfer function such as the sigmoid function is not applied at the processing nodes that serve as outputs. Therefore, for regression problems the output H_m is equal to the summed input of the m th processing node which serves as an output of the neural network being trained.

[Para 54] As described more fully below, in the case of a multi-output neural network the difference between actual output produced by the k th training data input, and the expected output is computed for each output of the neural network.

[Para 55] In block 712 the derivatives with respect to each of the weights in the neural network, of a k th term (corresponding to the k th set of training data) of an objective function being used to train the neural network are computed. Optimizing, and preferably, in particular minimizing, the objective function in terms of the weights is tantamount to training the neural network. In the case of a single output neural network the square of the difference given by Equation Four is preferably used in the objective function to be minimized. For a single output neural network the objective function is preferably given by:

EQU. 5

$$OBJ = \frac{1}{2N} \sum_{k=1}^N (H_m(\mathbf{W}, \mathbf{V}, \mathbf{X}_k) - Y_k)^2$$

[Para 56] where the summation index k specifies a training data set; and

[Para 57] N is the number of training data sets.

[Para 58] Alternatively, a different function of the difference is used as the objective function. The derivative of the k th term of the objective function given by Equation Five with respect to a weight of a directed edge coupling a i th input of the neural network to an j th processing node of the neural network is:

EQU. 6

$$\left. \frac{\partial OBJ}{\partial W_{ji}} \right|_k = \Delta R_k \frac{\partial H_m}{\partial W_{ji}}$$

[Para 59] The derivative on the right hand side of Equation Six which is the derivative of the summed input H_m at the m th processing node (which is the output node of the neural network) with respect to the weight W_{ji} of the neural network is unfortunately, for certain values of i, j , a rather complicated expression. This is due to the fact that the directed edge that is characterized by weight W_{ji} may be remote from the output (m th) node, and consequently a change in the value of W_{ji} can cause changes in the strength of signals reaching the m th processing node through many different signal paths (each including a series of one or more directed edges).

[Para 60] FIG. 8 shows four subgraphs including a first subgraph 802 that has two nodes, a second subgraph 804 that has three nodes, a third subgraph 806 that has four nodes, and a fourth subgraph 808 that has five nodes. The four subgraphs 802, 804, 806, 808 taken together illustrate the dependence of the number of different paths between two nodes on the number of nodes by which the two nodes are separated. The first subgraph 802 includes a first node 810 and a second node 812 that are connected together by a single (first) directed edge 814 which constitutes a single path.

[Para 61] Each successive subgraph (with the subgraphs 802–808 taken from left to right) can be understood as including a preceding subgraph (to its left) as a subgraph. As indicated by common reference numerals 810–814, the second subgraph 804 includes the first subgraph 802 as a subgraph. The second subgraph 804 also includes an additional, third node 816, a second directed edge 818, and a third directed edge 820. The second directed edge

818 connects the third node 816 to the first node 810 thereby accessing the single path of the first subgraph 802 which is a subgraph in the second subgraph 804. The third directed edge 820 couples the third node 816 directly to the second node 812 thereby providing an additional signal path. Thus, in the second subgraph 804 there is one signal path inherited from the first subgraph 802, and the path through the third directed edge 820 for a total of two paths between third node 816 and the second node 812.

[Para 62] As indicated again by common reference numerals the third subgraph 806 includes the second subgraph 804 as a subgraph. The third subgraph 806 includes an additional, fourth node 822, a fourth directed edge 824, a fifth directed edge 826, and a sixth directed edge 828. The fourth directed edge 824 connects the fourth node 822 to the third node 816, at which signal flow in the second subgraph 804 (here a subgraph) commences. Thus, the fourth directed edge 824 accesses the two signal paths of the second subgraph 804. The fifth directed edge 826 connects the fourth node 822 to the first node 810 at which signal flow in the first subgraph 802 (here a subgraph) commences, thus the fifth directed edge 826 provides access to an additional signal path. Finally, the sixth directed edge 828 provides a new signal path from the fourth node 822 directly to the second node 812, at which signal flow terminates in the third subgraph 806. Thus in the third subgraph 806 there are a total of $2+1+1=4$ signal paths between the fourth node 822 and the second node 812, which are separated by two interceding nodes in the third subgraph 806.

[Para 63] As indicated once more by common reference numerals the fourth subgraph 808 includes the third subgraph 806 as a subgraph. The fourth subgraph 808 also includes a fifth node 830, a seventh directed edge 832, an eighth directed edge 834, a ninth directed edge 836, and a tenth directed edge 838. The seventh directed edge 832 connects the fifth node 830 to the fourth node 822 at which signal flow for the third subgraph 806 (here a subgraph) commences, thereby accessing the four signal paths of the third subgraph 806. Similarly, the eighth directed edge 834 connects the fifth node 830 directly to the third node 816, thereby providing separate access to the

two signal paths of the second subgraph 804. The ninth directed edge 836 connects the fifth node 830 to the first node 810 thereby accessing the single signal path of the first subgraph 802. The tenth directed edge 838 directly connects the fifth node 830 to the second node 812 providing a separate signal path. Thus the number of signal paths between the fifth node 830 and the second node 812 is the sum of the signal paths from the first subgraph 802 (=1), the second subgraph 804 (=2), and the third subgraph 806 (=4), plus one for the tenth directed edge 838, which equals eight.

[Para 64] The five nodes 810, 812, 814, 816, 822, 830 have been enumerated in the order that they were introduced in the discussion above. However, according to the usual convention, the nodes are assigned successive integers proceeding in the direction of signal propagation, as is done in connection with FIG. 1 for the processing nodes 110–116. Based on the pattern of dependence of the number of signal paths on the number of nodes in the subgraph that is manifested in the four subgraphs 802–808 of FIG. 8, a general rule that relates the number of signal paths between two nodes to the separation between the two nodes can be deduced. Given the aforementioned conventional enumeration, the rule is expressed as:

EQU. 7

$$SP = 2^{m-k-1}$$

where SP is the number of signal paths;
m is the integer index of a signal sink node; and
k is the integer index of a signal source node.

[Para 65] To fully take into account the effect of signals propagating through all paths, on the derivatives in the right hand side of Equation Six, these derivatives can be evaluated for various values of i, j using the following generalized procedure expressed in pseudo code.

[Para 66] FIRST OUTPUT DERIVATIVE PROCEDURE:

If $j == m$,

$$\frac{\partial H_m}{\partial W_{mi}} = X_i$$

Otherwise,

$$w_j = X_i \frac{dT_j}{dH_j}$$

$$\frac{\partial H_m}{\partial W_{ji}} = V_{mj} w_j$$

For ($r=j+1$; $r<m$; $r++$)

{

$$w_r = \frac{dT_r}{dH_r} \sum_{t=j}^{r-1} V_{rt} w_t$$

$$\frac{\partial H_m}{\partial W_{ji}} + = V_{mr} w_r$$

}

[Para 67] In the first output derivative procedure

dT_r/dH_r is the derivative of the transfer function of an r th processing node treating the summed input H_r as an independent variable;
 dT_j/dH_j is the derivative of the transfer function of a j th processing node treating the summed input H_j as an independent variable; and
 w_j and w_r are temporary variables, used for holding incremental calculations.

[Para 68] The latter two derivatives dT_r/dH_r , dT_j/dH_j , are evaluated at the values of H_j and H_r that occur when a specific training data set (e.g., the k th) is propagated through the neural network being trained.

[Para 69] The sigmoid function given by Equation Two above has the property that its derivative is simply given by:

EQU. 8

$$\frac{dT_j}{dH_j} = h_j(1 - h_j)$$

where h_j is the output of a j th processing node that uses the sigmoid transfer function; and

H_j is the summed input of the j th processing node.

[Para 70] Therefore, in the case that the sigmoid function is used as the transfer function in processing nodes, the derivatives of the transfer function appearing in the first output derivative procedure are preferably replaced by the form given by Equation Eight. As mentioned above the output of each processing node (e.g., h_j) is determined and stored when training data is propagated through the neural network in step 708, and is thus available for use in the case that Equation Eight is used in the first derivative output procedure (or in the second derivative output procedure described below). In the alternative case of a transfer function other than the sigmoid function, in which the derivatives of transfer function are expressed in terms of the independent variable (input to transfer function), it is appropriate when propagating training data through the neural network, in block 708, to determine and store, at least temporarily, the summed input to each processing node, so that such input can be used in evaluating derivatives of processing nodes transfer functions in the course of executing the first output derivative procedure.

[Para 71] Although the working of the first output derivative procedure is more concisely and effectively communicated via the pseudo code shown above than can be communicated in words, a description of the procedure is as follows. In the special case that the weight under consideration connects to the output under consideration (i.e., if $j=m$), then the derivative of the summed input H_m with respect to the weight W_{ji} is simply set to the value of the i th input X_i , because the contribution to H_m that is due to the input W_{ji} is simply the product of X_i and W_{ji} .

[Para 72] In the more complicated and more common case in which the directed edge characterized by the weight W_{ji} under consideration is not directly connected to the output (m th) node under consideration the procedure works as follows. First, an initial contribution to the derivative being calculated that is related to a weight V_{mj} is computed. The weight V_{mj}

characterizes a directed edge that connects the j th processing node at which the directed edge characterized by the weight W_{ji} with respect to which the derivative is being taken terminates, to the m th output, the derivative of the summed input of which, is to be calculated. The initial contribution includes a first factor that is the product of the derivative of the transfer function of the j th node at which the weight W_{ji} terminates (evaluated at its operating point given a set of training data), and the input X_i at the i th input, at which the directed edge characterized by the weight W_{ji} originates, and a second factor that is the weight V_{mj} . The first factor which is aptly termed a leading part of the initial contribution is stored and will be used subsequently. The initial contribution is a summand which will be added to as described below.

[Para 73] After the initial contribution has been computed, the *for* loop in the pseudo code listed above is entered. The *for* loop considers successive r th processing nodes, starting with the $(j+1)$ th node that immediately follows the j th node at which the directed edge characterized by the W_{ji} weight with respect to which the derivative being taken terminates, and ending at the $(m-1)$ node immediately preceding the output (m th) node under consideration, the summed input of which the derivative being taken is of. At each r th node another r th summand–contribution to the derivative is computed. The contribution of each r th processing node in the range $j+1$ to $m-1$ includes a leading part that is the product of the derivative of the transfer function of the node in question (r th) at its operating point, and what shall be called an r th intermediate sum. The r th intermediate sum includes a term for each t th processing node from the j th processing node up to the $(r-1)$ th node that precedes the r th processing node for which the intermediate sum is being evaluated. For each t th node of the aforementioned sequence of nodes j th to $(r-1)$ th the summand of the r th intermediate sum is a product of a weight characterizing a directed edge from the t th processing node to the r th processing node, and the value of the leading part that has been calculated during a previous iteration of the *for* loop for the t th processing node (or in the case of the j th node calculated before entering the *for* loop). The leading parts can thus be said to be calculated in a recursive manner in the first output derivative procedure. Furthermore, in the each r th summand contribution to

the overall derivative being calculated, the aforementioned leading part for the r th node, and a weight that characterizes a directed edge from the r th node to the m th processing node are multiplied together.

[Para 74] The first output derivative procedure could be evaluated symbolically for any values of j , i , and m for example by using a computer algebra application such as Mathematica, published by Wolfram Research of Champaign, IL in order to present a single closed form expression. However, in as much as numerous sub-expressions (i.e., the above mentioned leading parts) would appear repetitively in such an expression, it is more computationally efficient and therefore preferable to evaluate the derivatives given by the first output derivative procedure using a program that is closely patterned after the pseudo code representation.

[Para 75] The derivative of the k th term of the objective function given by Equation Five with respect to a weight V_{dc} of a directed edge coupling the output of a c th processing node to the input of a d th processing node is:

EQU. 9

$$\left. \frac{\partial OBJ}{\partial V_{dc}} \right|_k = \Delta R_k \frac{\partial H_m}{\partial V_{dc}}$$

[Para 76] The derivative on the right side of Equation Nine is the derivative of the summed input an m th processing node that serves as an output of the neural network with respect to a weight that characterizes the directed edge that couples the c th processing node to the d th processing node. This derivative can be evaluated using the following generalized procedure expressed in pseudo code:

[Para 77] SECOND OUTPUT DERIVATIVE PROCEDURE:

If $d==m$,

$$\frac{\partial H_m}{\partial V_{mc}} = h_c$$

Otherwise,

$$v_d = h_c \frac{dT_d}{dH_d}$$

$$\frac{\partial H_m}{\partial V_{dc}} = V_{md} v_d$$

For (r=d+1; r<m; r++)

{

$$v_r = \frac{dT_r}{dH_r} \sum_{t=d}^{r-1} V_{rt} v_t$$

$$\frac{\partial H_m}{\partial V_{dc}} + = V_{mr} v_r$$

}

[Para 78] The second output derivative procedure is analogous to the first output derivative procedure. In the preferred case that the transfer function of processing nodes in the neural network is the sigmoid function, in accordance with Equation Eight, dT_r/dH_r is replaced by $h_r(1-h_r)$, and dT_d/dH_d is replaced by $h_d(1-h_d)$. v_r and v_d are temporary variables. The exact nature of second output derivative procedure is also evident by inspection. The second output derivative procedure functions in a manner analogous to the first output derivative procedure.

[Para 79] Although the exact nature of the second derivative output procedure is, as in the case of the first derivative procedure, best ascertained by examining the pseudo code presented above, the operations can be described as follows: In the special case that the weight under consideration characterizes a directed edge that connects to the output under consideration (i.e., if $d=m$), then the derivative of the summed input H_m with respect to the weight V_{dc} is simply set to the value of the output h_c of the c th processing node at which the directed edge characterized by the weight V_{dc} with respect to which the derivative being calculated originates, because the contribution to H_m that is due to the input V_{dc} is simply the product of V_{dc} and h_c .

[Para 80] In the more complicated and more common case in which the directed edge characterized by the weight under consideration is not directly

connected to the m th output under consideration the procedure works as follows. First, an initial contribution to the derivative being calculated that is due to a weight V_{md} is computed. The weight V_{md} characterizes a directed edge that connects the d th processing node at which the directed edge characterized by the weight V_{dc} with respect to which the derivative is being taken, terminates, to the m th output the derivative of the summed input of which is to be calculated. The initial contribution includes a first factor that is the product of the derivative of the transfer function of the d th node at which the weight V_{dc} terminates (evaluated at its operating point given a set of training data input), and the output h_c at the c th processing node, at which the directed edge characterized by the weight V_{dc} originates, and a second factor that is the weight V_{md} that characterizes a directed edge between the d th and m th nodes. The first factor which is aptly termed a leading part of the initial contribution is stored and will be used subsequently. The initial contribution is a summand which will be added to as described below.

[Para 81] After the initial contribution has been computed, the *for* loop in the pseudo code listed above is entered. The operation of the *for* loop in the second output derivative procedure is analogous to the operation of the *for* loop in the first output derivative procedure that is described above.

[Para 82] Equation Seven which enumerates the number of paths between two nodes in a generalized feed forward neural network suggests that the computational cost of evaluating the derivatives in the right hand sides of Equations Six and Nine would be proportional to two raised to the power of one less than the difference between an index (m) identifying a node at which output is taken and an index (j or d) which identifies a node at which a directed edge characterized by the weight with respect to which the derivative is taken terminates. However, by using the first and second output derivative procedures, in which the leading parts are saved and reused, the computation cost of calculating the derivatives in the right hand sides of Equations Six and Nine is reduced to:

EQU. 10

$$CC \propto \frac{1}{2} n(n+1)$$

where, CC is the computational cost; and
n is equal to the difference m–k of the indices defined in the context
of Equation Seven.

[Para 83] For certain applications, it is desirable to provide a large number of processing nodes. Although, using the first and second derivative output procedures reduces the computational cost of evaluating derivatives, even if these are used the computational cost rises rapidly as the number of processing nodes is increased.

[Para 84] A highly accurate, method of estimating the derivatives appearing in the right hand sides of Equation Six and Nine has been determined. This method has a lower computational cost than the first and second output derivative procedures. In fact, the computational cost is linear in n, the variable appearing in Equation Ten. An analysis that elucidates why the estimation method is as accurate as it is, is given below as an introduction to the method.

[Para 85] Consider a feed forward neural network in which the transfer function of each node is the sigmoid function. The derivative of a summed input H_m to an m^{th} output node with respect to a weight characterizing a directed edge from an i^{th} node to a k^{th} node includes a term that is based on signal flow along a path that passes through each node between the k^{th} node and the m^{th} node. This term is given by the following product:

EQU. 11

$$V_{m,m-1} \bar{h}_{m-1} \cdot V_{m-1,m-2} \bar{h}_{m-2} \cdot \dots \cdot V_{k+1,k} \bar{h}_k \frac{\partial H_k}{\partial W_{ki}} = \left(\prod_{r=k}^{m-1} V_{r+1,r} \right) \left(\prod_{r=k}^{m-1} \bar{h}_r \right) \cdot \frac{\partial H_k}{\partial W_{ki}}$$

[Para 86] In Equation Eleven

\bar{h}_x

is the value of the derivative of the transfer function of an x^{th} node. In the right hand side of Equation Eleven, the product of weights of directed edges along the path have been collected, and the product of the derivatives of the transfer functions encountered along the path have been collected. It is of consequence that the derivative of

the sigmoid transfer function takes on a maximum value of 0.25. (The exact value of 0.25 is obtained when the independent variable is equal to zero). The maximum value of the derivative the sigmoid transfer function determines an upper bound on the term of the derivative given in Equation Eleven that is expressed as:

EQU. 12:

$$\left| \left(\prod_{r=k}^{m-1} V_{r+1,r} \right) \left(\prod_{r=k}^{m-1} h_r \right) \cdot \frac{\partial H_k}{\partial W_{ki}} \right| \leq \frac{1}{4^{m-k}} \left| \left(\prod_{r=k}^{m-1} V_{r+1,r} \right) \frac{\partial H_k}{\partial W_{ki}} \right|$$

[Para 87] It has been observed that most directed edge weights in a well trained feed forward neural network of the type shown in FIG. 1 are in the range (0,1). Based on this it is reasonable to assume that the remaining product in the right hand side of Equation Twelve is less than one. Accordingly, the upper bound on the derivative term shown in Equation Eleven can be rewritten as:

EQU. 13

$$\left| \left(\prod_{r=k}^{m-1} V_{r+1,r} \right) \left(\prod_{r=k}^{m-1} h_r \right) \cdot \frac{\partial H_k}{\partial W_{ki}} \right| \leq \frac{1}{4^{m-k}} \left| \frac{\partial H_k}{\partial W_{ki}} \right|$$

[Para 88] Equation Thirteen demonstrates that the contribution of a path from a directed edge characterized by a weight with respect to which the derivative is being taken, to the derivative in question decreases by at least 75% for each additional directed edge along the path. In other words, paths that include many directed edges contribute little to the derivative in question.

[Para 89] The preceding arguments, presented with reference to Equations 11–13 provide an ex post facto explanation of why derivative estimation procedures described below are as accurate as they are.

[Para 90] A first derivative estimation procedure that can be used to estimated the derivative of an input H_m to an m^{th} output node with respect to a weight W_{ki} characterizing a directed edge from an i^{th} input to a k^{th} node is expressed in pseudo code as:

[Para 91] FIRST DERIVATIVE ESTIMATION PROCEDURE

If $k==m$,

$$\frac{\partial H_m}{\partial W_{mi}} = X_i$$

Otherwise,

$$w_k = X_i \frac{dT_k}{dH_k}$$

$$\frac{\partial H_m}{\partial W_{ki}} = V_{mk} w_k$$

For ($r=k+1$; $r<m$; $r++$)

$$\left\{ \begin{array}{l} \frac{\partial H_m}{\partial W_{ki}} += V_{mr} V_{rk} \frac{dT_r}{dH_r} w_k \end{array} \right.$$

[Para 92] Although, the exact nature of the first derivative estimation procedure is best ascertained by examining the pseudo code representation given above, the first derivative estimation procedure can be described in words as follows. First in the special case that the directed edge, characterized by the weight with respect to which the derivative is being taken, terminates at the output node, the input of which is being differentiated the derivative being estimated is simply set equal to the value X_i of the input at the i^{th} input node at which the directed edge characterized by the weight with respect to which the derivative is being taken, originates. In this special case the procedure gives the exact value of the derivative.

[Para 93] In the more general case, a leading part denoted w_k which is the product of a signal X_i emanating from the i^{th} node at which the directed edge characterized by the weight with respect to which the derivative is being taken originates and the transfer function of a k^{th} node at which the directed edge characterized by the weight with respect to which the derivative is being taken terminates, is computed. Next an initial contribution to the derivative being estimated which is the product of the leading part and a weight of a directed edge from the k^{th} node to the m^{th} output node is calculated. The initial

contribution is a summand to which a summand for each node between the k^{th} node and the m^{th} node is added. For each r^{th} node between the k^{th} node and the m^{th} node a summand that is the product of a weight of a directed edge from the k^{th} node to the r^{th} node, a weight of a directed edge from the r^{th} node to the m^{th} node, a transfer function of the r^{th} node, and the leading part denoted w_k is added. Note that each of these summands for each r^{th} node involves a path that includes only two directed edges.

[Para 94] Similar to the first derivative estimation procedure, a second derivative estimation procedure that can be used to estimated the derivative of an input H_m to an m^{th} output node with respect to a weight V_{cd} characterizing a directed edge from a c^{th} processing node to a d^{th} node is expressed in pseudo code as:

[Para 95] SECOND DERIVATIVE ESTIMATION PROCEDURE

 If $d==m$,

$$\frac{\partial H_m}{\partial V_{mc}} = h_c$$

 Otherwise,

$$v_d = h_c \frac{dT_d}{dH_d}$$

$$\frac{\partial H_m}{\partial V_{dc}} = V_{md} v_d$$

 For ($r=d+1$; $r<m$; $r++$)

$$\left\{ \begin{array}{l} \frac{\partial H_m}{\partial V_{dc}} + = V_{mr} V_{rd} \frac{dT_r}{dH_r} v_d \end{array} \right.$$

[Para 96] The second derivative estimation procedure is the same as the first derivative estimation procedure, with the exception that the input X_i is replaced by the output h_i of the i^{th} node at which the directed edge, that is characterized by the weight with respect to which the derivative being evaluated is taken, originates.

[Para 97] The first and second derivative estimation procedures only consider paths that have at most two directed edges between a node at which a directed edge characterized by the weight with respect to which a derivative being taken terminates and an output node. Other paths that are made up of more directed edges are ignored. Nonetheless, the first and second derivative estimation procedures give very accurate estimates.

[Para 98] In the case that the transfer function of processing nodes in the neural network is the sigmoid function, the form of the derivative of the sigmoid transfer function given in Equation Eight is suitably used in the first and second derivative estimation procedures.

[Para 99] FIG. 9 illustrates four subgraphs including a first subgraph 902 that has two nodes, a second subgraph 904 that has three nodes, a third subgraph 906 that has four nodes and a fourth subgraph 908 that has five nodes. These subgraphs are similar to the four subgraphs shown in FIG. 8. However, the subgraphs shown in FIG. 9 include only those directed edges that are involved in paths that are considered in the first and second derivative estimation procedures, in the case that a derivative of a summed input to the bottom node of each subgraph with respect to a weight characterizing a directed edge that terminates at the top node in each subgraph is being estimated. Note that only paths that involve one or two directed edges are shown in FIG. 9.

[Para 100] To demonstrate the accuracy of the first and second derivative estimation procedures a numerical experiment was performed. The numerical experiment involved a neural network of the type shown in FIG. 1 that had two inputs, (one of which would be used to input a bias signal), five processing nodes and one output. The output was taken from the output of the summer of the fifth processing node. Weights characterizing the directed edges in the neural networks were selected using a random number generator. The randomly generated weights are shown in FIG. 10. The arrangement of FIG. 10 is the same as that of FIG. 3, described above. A bias of value of 1 and an input value of -3 were assumed. The derivative of the output with respect to each weight was then calculated using the first and second output derivative

procedures, and then recalculated using the first and second derivative estimation procedures. The results obtained using the first and second output derivative procedures are shown in FIG. 11. The results obtained using the first and second derivative estimation procedure are shown in FIG. 12. In FIGs. 10, 11 the derivatives are arranged in the same arrangement as the weights are arranged in FIG. 10. As is evident in FIGs. 10–11 the results only differ in the third significant figure for three derivatives that are affected by the approximation.

[Para 101] Thus, in calculating the derivatives in block 712 of the process shown in FIG. 7, either the first and second output derivative procedures or the first and second derivative estimation procedures are alternatively used. The lower computational cost of the first and second derivative estimation procedures would weigh in favor of using them as the number of nodes of a neural network is increased.

[Para 102] Referring again to FIG. 7, in step 714 the derivatives calculated in the preceding step 712 are stored. The next block 716 is a decision block the outcome depends on whether there are more sets of training data to be processed. If affirmative then in block 718 a counter that points to successive training data sets is incremented, and thereafter the process 700 returns to block 706. Thus, blocks 706 to 714 are repeated for a plurality of sets of training data. If in block 716 it is determined that all of the training data sets have been processed, then the method 700 continues with block 720 in which the derivatives with respect to each weight are averaged over the training data sets. The average over N training data sets of the derivative of the objective function with respect to the weight characterizing a directed edge from an i th input to a j th processing node is given by:

EQU. 14

$$AVG\left(\frac{\partial OBJ}{\partial W_{ji}}\right) = \frac{1}{N} \sum_{k=1}^N \Delta R_k \frac{\partial H_m}{\partial W_{ji}}$$

[Para 103] Similarly, the average over N training data sets of the derivative of the objective function with respect to the weight characterizing a directed edge from cth processing node to dth processing node is given by:

EQU. 15

$$AVG\left(\frac{\partial OBJ}{\partial V_{dc}}\right) = \frac{1}{N} \sum_{k=1}^N \Delta R_k \frac{\partial H_m}{\partial V_{dc}}$$

[Para 104] Note that the derivatives $\partial H_m / \partial W_{ji}$, $\partial H_m / \partial V_{dc}$ in the right hand sides of Equations Fourteen and Fifteen must be evaluated separately for each kth set of training data, because they are dependent on the operating point of the transfer function block (e.g. 206) in each processing node which is dependent on the training data applied to the neural network.

[Para 105] In step 722 the average of the derivatives of the objective function that are computed in step block 720 are processed with an optimization algorithm in order to calculate new values of the weights. Depending on how the objective function to be optimized is set up, the optimization algorithm seeks to minimize or maximize the objective function. The objective function given in Equation Five and other objective functions shown herein below are set up to be minimized. A number of different optimization algorithms that use derivative evaluation including, but not limited to, the steepest descent method, the conjugate gradient method, or the Broyden–Fletcher–Goldfarb–Shanno method are suitable for use in block 722. Suitable routines for use in step 722 are available commercially and from public domain sources. Suitable routines that implement one or more of the above mentioned methods or other suitable gradient based methods are available from the Netlib a World Wide Web accessible repository of algorithms, and commercially from, for example, Visual Numerics of San Ramon, Ca. Algorithms that are appropriate for step 722 are described, for example, in chapter 10 of the book “Numerical Recipes in Fortran” edited by William H. Press, and published by the Cambridge University Press and in chapter 17 of the book “Numerical Methods That Work” authored by Forman S. Acton, and published by Harper & Row. Although the intricacies of nonlinear optimizations routines are outside of the focus of the present description, an outline of the application of the steepest descent

method is described below. Optimization routines that are structured for reverse communication are advantageously used in step 722. In using an optimization routine that uses reverse communication, the optimization routine is called (i.e., by a routine that embodies method 700) with values of derivatives of a function to be optimized.

[Para 106] In the case that the steepest descent method is used in step 722, a new value of the weight that characterizes the directed edge from the i th input to the j th processing node is given by:

EQU. 16

$$W_{ji}^{new} = W_{ji}^{old} - \alpha AVG \left(\frac{\partial OBJ}{\partial W_{ji}} \right)$$

where, α is a step length control parameter.

[Para 107] Also using the steepest descent method a new value of the weight that characterizes the directed edge from the c th processing node to the d th processing node is given by:

EQU. 17

$$V_{dc}^{new} = V_{dc}^{old} - \beta AVG \left(\frac{\partial OBJ}{\partial V_{dc}} \right)$$

where β is a step length control parameter.

[Para 108] The step length control parameters are often determined by the optimization routine employed, although in some cases the user may effect the choice by an input parameter.

[Para 109] Although, as described above, new weights are calculated using derivatives of the objective function that are averaged over all N training data sets, alternatively new weights are calculated using averages over less than all of the training data sets. For example, one alternative is to calculate new weights based on the derivatives of the objective function for each training data set separately. In the latter embodiment it is preferred to cycle through the available training data calculating new weight values based on each training data set.

[Para 110] Block 724 is a decision block the outcome of which depends on whether a stopping condition is satisfied. The stopping condition preferably requires that the difference between the value of the objective function evaluated with the new weights and the value of the objective function calculated with the old weights is less than a predetermined small number, that the Euclidean distance between the new and the old processing node to processing node weights is less than a predetermined small number, and that the Euclidean distance between the new and old input-to-processing node weights is less than a predetermined small value. Expressed in mathematical notation the preceding conditions are:

EQU. 18

$$|OBJ^{NEW} - OBJ^{OLD}| < \epsilon_1$$

EQU. 19

$$\|W^{OLD} - W^{NEW}\| < \epsilon_2$$

EQU. 20

$$\|V^{OLD} - V^{NEW}\| < \epsilon_3$$

W^{NEW} , W^{OLD} are collections of the weights that characterize directed edges between inputs and processing nodes that were returned by the last call and the call preceding the last call of the optimization algorithm respectively.

V^{NEW} , V^{OLD} are collections of the weights that characterize directed edges between processing nodes that were returned by the last call and the call preceding the last call of the optimization algorithm respectively. The collections of weights are suitably arranged in the form of a vector for the purpose of finding the Euclidean distances.

OBJ^{NEW} and OBJ^{OLD} are the values of the objective function e.g., Equation Five for the current and preceding values of the weights.

[Para 111] The predetermined small values used in the inequalities Eighteen through Twenty can be the same value. For some optimization routines the predetermined small values are default values that can be overridden by a call parameter.

[Para 112] If the stopping condition is not satisfied, then the process 700 loops back to block 704 and continues from there to update the weights again as described above. If on the other hand the stopping condition is satisfied then the process 700 continues with block 730 in which weights that are below a certain threshold are set to zero. For a sufficiently small threshold, setting weights that are below that threshold to zero has a negligible effect on the performance of the neural network. An appropriate value for the threshold used in step 730 can be found by routine experimentation, e.g., by trying different values and judging the effect on the performance of one or more neural networks. If certain weights are set to zero the directed edges with which they are associated need not be provided. Eliminating directed edges simplifies the neural network and thereby reduces the complexity and semiconductor die space required for hardware implementations of the neural network. Alternatively, step 730 is eliminated. After process 700 has finished or after process 800 (described below) has been completed if the latter is used, the final values of the weights are used to construct a neural network. The neural network that is constructed using the weights can be a software implemented neural network that is for example executed on a Von Neumann computer; however, it is alternatively a hardware implemented neural network. The weights found by the training process 700 are built into an actual neural network that is to be used in processing input data and producing output.

[Para 113] Method 700 has been described above with reference to a single output neural network. Method 700 is alternatively adapted to training a multi-output neural network of the type illustrated in FIG. 1. For multi-output neural networks that are used for regression or other problems with continuous outputs, in lieu of the objective function of Equation Five, an objective function of the following form is preferred:

EQU. 21

$$OBJ = \frac{1}{2MP} \sum_{t=1}^P \sum_{k=1}^M (H_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_k) - Y_{kt})^2$$

where the summation index k specifies a particular set of training data;

the summation index t specifies a particular output;

P is the number of output processing nodes;

M is the number of training data sets;

$H_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_k)$ is the output (equal to the summed input) at a t th processing node when a k th vector of training data input is applied to the neural network; and

Y_{kt} , is the expected output value for the t th processing node that is associated with the k th set of training data.

[Para 114] Equation Twenty-One is particularly applicable to neural networks for multi-output regression problems. As noted above for regression problems it is preferred not to apply a threshold transfer function such as the sigmoid function at processing nodes that serve as the outputs. Therefore, the output at each t th output processing node is preferably simply the summed input to that t th output processing node.

[Para 115] Equation Twenty-One averages the difference between actual outputs produced in response a training data and the expected outputs associated with the training data. The average is taken over the multiple outputs of the neural network, and over multiple training data sets.

[Para 116] The derivative of the latter objective function with respect to a weight of the neural network is given by:

EQU. 22

$$\frac{\partial OBJ}{\partial w_i} = \frac{1}{MP} \sum_{k=1}^M \left(\sum_{t=1}^P (H_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_k) - Y_{kt}) \frac{\partial H_t}{\partial w_i} \right)$$

where w_i stands for either a weight characterizing input-to-processing node directed edges, or directed edges that couple processing nodes.

(Note that because H_t is a function of k , the derivative $\partial H_t / \partial w_i$ must be evaluated for each value of k separately.)

[Para 117] In the case of a multi-output neural network the weights are adjusted based on the effect of the weights on all of the outputs. In an adaptation of the process shown in FIG. 7 to a multi-output neural network derivatives of the form shown in Equation Twenty-Two, that are taken with respect to each of the weights in the neural network to be determined, are processed by an optimization algorithm in step 722.

[Para 118] In addition to the control application mentioned above, an application of multi-output neural networks of the type shown in FIG. 1, is to predict the high and low values that occur during a k th period of finite duration of stochastic times series data (e.g., stock market data) based on input high and low values for n preceding periods $(k-n)$ to $(k-1)$.

[Para 119] As mentioned above in classification problems it is appropriate to apply the sigmoid function at the output nodes. (Alternatively, other threshold functions are used in lieu of the sigmoid function.) Aside from the special case in which what is desired is a yes or no answer as to whether a particular input belongs to a particular class, it is appropriate to use a multi-output neural network of the type shown in FIG. 1 to solve classification problems.

[Para 120] In classification problems one way to represent an identification of a particular class for an input vector, is to assign each of a plurality of outputs of the neural network to a particular class. An ideal output for such a network, might be an output value of one at the neural network output that correctly corresponds to the class of an input vector, and output values of zero at each of the remaining neural network outputs. In practice, the class associated with the neural network output node at which the highest value is output in response to a given input vector is construed as the correct class for the input vector. In the alternative, the neural network is trained to output a low value

(ideally zero) at an output corresponding to the correct class, and output values close to one (ideally one) at other outputs.

[Para 121] For multi-output classification neural networks an objective function of the following form is preferable:

EQU. 23

$$R(\mathbf{W}, \mathbf{V}) = \frac{1}{2MP} \sum_{k=1}^M \sum_{t=1}^P \Delta R_{kt}^2$$

where, the t summation index specifies output nodes of the neural network;

the k summation index identifies a training data set with which actual and expected outputs are associated; and

EQU. 24

$$\Delta R_{kt} = \begin{cases} h_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_k) - Y_{kt} & \text{for wrong classification} \\ 0 & \text{for correct classification} \end{cases}$$

where h_t is the output of the a transfer function at a tth processing node that serves as an output of the neural network.

[Para 122] Equation Twenty-Four is applied as follows. For a given k th set of training data, in the case that the correct output of the neural network being trained has the highest value of all the outputs of the neural network (even though it is not necessarily equal to one), the output for that k th training data is treated as being completely correct and ΔR_{KT} is set to zero for all outputs from 1 to P. If the correct output does not have the highest value, then element by element differences are taken between the actual output produced in response to the k th training data input and expected output that is associated with the k th training data set.

[Para 123] Such a neural network is preferably trained with training data sets that include input vectors for each of the classes that are to be identified by the neural network.

[Para 124] The derivative of the objective function given in Equation Twenty-Three with respect to an k th weight of the neural network is:

EQU. 25

$$\frac{\partial OBJ}{\partial w_i} = \frac{1}{MP} \sum_{k=1}^M \left(\sum_{t=1}^P \Delta R_{kt} \frac{dT_t}{dH_t} \frac{\partial H_t}{\partial w_i} \right)$$

where dT/dH_t is the derivative of the transfer function of the t th processing node with respect to the summed input H_t . of the t th processing node (with the summed input treated as an independent variable)

[Para 125] In the preferred case that the transfer function is the sigmoid function the derivative dh_t/dH_t can be expressed as $h_t(1-h_t)$ where h_t is the value of the sigmoid function for summed input H_t . In an adaptation of the process shown in FIG. 7 to a multi-output neural network used for classification, derivatives of the form shown in Equation Twenty-Five, that are taken with respect to each of the weights in the neural network to be determined, are processed by the optimization algorithm in step 722.

[Para 126] It is desirable to reduce the number of directed edges in neural networks of the type shown in FIG. 1. Among the benefits of reducing the number of directed edges is a reduction in complexity, and power dissipation of hardware implemented embodiments. Furthermore, neural networks with fewer interconnections are less prone to over-training. Because it has learned the specific data but not their underlying structure, an over-trained network performs well with training data but not with other data of the same type to which it is applied subsequent to training. According to further embodiments of the invention described below, a cost term that is dependent on the number of weights of significant magnitude is included in an objective function used in training with an aim of reducing the number of weights of significant magnitude. A predetermined scale factor is used to judge the size of weights. Recall that in step 730 discussed above, directed edges characterized by weights that are below a predetermined threshold are preferably excluded from implemented neural networks. Using an objective function that tends to reduce the number of weights of significant magnitude in combination with step 730 tends to reduce the complexity of neural networks produced by the training method 700.

[Para 127] Preferably the aforementioned cost term is a continuously differentiable function of the magnitude of weights so that it can be included in an objective function that is optimized using optimization algorithms, such as those mentioned above, that require derivative information.

[Para 128] A preferred continuously differentiable expression of the number of near zero weights in a neural network is:

EQU. 26

$$U = \sum_{i=1}^K e^{-\eta w_i^2}$$

where w_i is an i th weight of the neural network; and η is a scale factor relative to which the magnitude of weights are judged.

η is preferably chosen such that if a weight is equal to the threshold used in step 730 below which weights are set to zero, the value of the summand in Equation Twenty-One is preferably at least 0.5.

[Para 129] The summation in Equation Twenty-Six preferably includes all the weights of the neural network that are to be determined in training.

Alternatively, the summation is taken over a subset of the weights.

[Para 130] The expression of near-zero weights is suitably normalized by dividing by the total number of possible weights for a network of the type shown in FIG. 1 which number is given by Equation One above. The normalized expression of the number of near zero weights is given by:

EQU. 27

$$F = \frac{U}{K}$$

F can take on values in the range from zero to one. F or other measures of near zero weights are preferably included in an objective function along with a measure of the differences between actual and expected output values. In order that F can have a significant impact in reducing the number of weights of significant value, it is desirable that the value and the derivative of F is not

insubstantial compared with the measure of the differences between actual and expected output values. One preferred way to address this goal is to use the following measure of differences between actual and expected values of:

EQU. 28

$$L = \frac{R_N}{R_O + R_N}$$

where R_N is a measure of the differences between actual and expected values during a current iteration of the training algorithm; and

R_O is a value of the measure of differences between actual and expected values for an iteration of the training algorithm preceding the current iteration.

[Para 131] According to the above definition, L also takes on values in the range from zero to one. The measure of differences used in Equation Twenty-Eight is preferably the sum of the squares of differences between actual output produced by training data, and expected output values associated with training data.

[Para 132] An objective function that combines the normalized expression of the number of near zero weights and the measure of the differences between actual and expected values is:

EQU. 29

$$OBJ = (1 - \lambda)L - \lambda F$$

in which, λ is a user chosen parameter that determines the relative priority of the sub-objective of minimizing the differences between actual and expected values, and the sub-objective of minimizing the number of weights of significant value. λ is preferably chosen in the range of 0.01 to 0.1, and is more preferably approximately equal to 0.05. Too high a value of λ can lead to reduction of the complexity of the neural network at the expense of its prediction or classification performance, whereas too

low of a value can lead to a network that is excessively complex and in some cases prone to over training. Note that the normalized expression of the number of near zero weights F (Equation Twenty-Seven) appears with a negative sign in the objective function given in Equation Twenty-Nine, so that F serves as a term of the cost function that is dependent on the number of weights of significant value.

[Para 133] The derivative of the expression of the number of near zero weights given Equation Twenty-Seven with respect to an i th weight w_i is:

EQU. 30

$$\frac{\partial F}{\partial w_i} = -\frac{2\eta}{K} w_i e^{-\eta w_i^2}$$

and the derivative of the measure of differences between actual and expected values given by Equation Twenty-Eight with respect to an i th weight w_i is:

EQU. 31

$$\frac{\partial L}{\partial w_i} = \frac{R_o}{(R_o + R_N)^2} \frac{\partial R_N}{\partial w_i}$$

In evaluating the latter derivative, R_o is treated as a constant.

[Para 134] Adapting the form of the measure of differences between actual and expected values given in Equation Five (i.e., the average of squares of differences) and taking the derivative with respect to the i th weight w_i the following derivative of the objective function of Equation Twenty-Nine is obtained:

EQU. 32

$$\frac{\partial OBJ}{\partial w_i} = (1 - \lambda) \frac{R_o}{(R_o + R_N)^2} \frac{1}{N} \sum_{q=1}^N (H_m(\mathbf{W}, \mathbf{V}, \mathbf{X}_q) - Y_q) \frac{\partial H_m}{\partial w_i} + \frac{2\lambda\eta}{K} w_i e^{-\eta w_i^2}$$

where,

EQU. 33

$$R_N = \frac{1}{2N} \sum_{k=1}^N (H_m(\mathbf{W}, \mathbf{V}, \mathbf{X}_k) - Y_k)^2$$

the summation index q specifies one of N training data sets.

[Para 135] Similarly, by adapting the form of the measure of differences between actual and expected values given in Equation Twenty-One, which is appropriate for multi-output neural networks used for regression problems, and taking the derivative with respect to an ith weight w_i the following derivative of the objective function of Equation Twenty-Nine is obtained:

EQU. 34

$$\frac{\partial OBJ}{\partial w_i} = (1 - \lambda) \frac{R_o}{(R_o + R_N)^2} \frac{1}{MP} \sum_{q=1}^M \left(\sum_{t=1}^P (h_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_q) - Y_{qt}) \frac{\partial H_t}{\partial w_i} \right) + \frac{2\lambda\eta}{K} w_i e^{-\eta w_i^2}$$

where,

EQU. 35

$$R_N = \frac{1}{2MP} \sum_{q=1}^M \left(\sum_{t=1}^P (h_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_q) - Y_{qt})^2 \right)$$

the summation index q specifies one of M training data sets; and the summation index t specifies one of P outputs of the neural network.

[Para 136] Also, by adapting the form of the measure of differences between actual and expected values given in Equation Twenty-Three, which is appropriate for multi-output neural networks used for classification problems, and taking the derivative with respect to an ith weight w_i the following derivative of the objective function of Equation Twenty-Nine is obtained:

EQU. 36

$$\frac{\partial OBJ}{\partial w_i} = \frac{2\lambda\eta}{K} w_i e^{-\eta w_i^2} + (1 - \lambda) \frac{R}{(R_o + R_N)^2} \frac{1}{MP} \sum_{k=1}^M \sum_{t=1}^P \left[(h_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_k) - Y_{kt}) \frac{dT}{dH_t} \frac{\partial H_t}{\partial w_i} \right]$$

where,

EQU. 37

$$R_N = \frac{1}{2MP} \sum_{k=1}^M \sum_{t=1}^P (h_t(\mathbf{W}, \mathbf{V}, \mathbf{X}_k) - Y_{kt})^2$$

Note that in the Equations presented above h_t stands for the output of the tth node's transfer function which is preferably but not necessarily the sigmoid function.

[Para 137] By optimizing the objective functions of which Equations Thirty-Two, Thirty-Four and Thirty-Six are the required derivatives, and thereafter

setting weights below a certain threshold to zero, neural networks that perform well, are less complex and less prone to over training are generally obtained.

[Para 138] FIG. 13 is a flow chart of a process 1300 of selecting the number of nodes in neural networks of the types shown in FIGs. 1, 6 according to the preferred embodiment of the invention. The process 1300 shown in FIG. 3 seeks to find the minimum number of processing nodes required to achieve a prescribed accuracy. In block 1302 a neural network is set up with a number of nodes. The number of nodes can be a number selected at random or a number entered by a user based on the user's guess as to how many nodes might be required to solve the problem to be solved by the neural network. In block 1304 the neural network set up in block 1302 is trained until a stopping condition (e.g., the stopping condition described with reference to Equations Eighteen, Nineteen and Twenty) is realized. The training performed in block 1304 and in blocks 1310 and 1318 discussed below is preferably done according to the process shown in FIG. 7. Block 1306 is a decision block, the outcome of which depends on whether the performance of the neural network trained in step 1304 is satisfactory. The decision made in block 1306 (and those made in blocks 1312, and 1320 described below) is preferably an assessment of accuracy based on comparisons of actual output for training data, and expected output associated with the training data. For example, the comparison may be made based on the sum of the squares of differences.

[Para 139] If in block 1306 it is determined that performance of neural network is not satisfactory, then in order to try to improve the performance by adding additional processing nodes, the process 1300 continues with block 1308 in which the number of processing nodes is incremented. The topology of the type shown in FIG. 1 (i.e., a feed-forward sequence of processing nodes) is preferably maintained when incrementing the number of processing nodes. In block 1310 the neural network formed in the preceding block 1308 by incrementing the number of nodes is trained until the aforementioned stopping condition is met. Next, in block 1312 it is ascertained whether or not the performance of the augmented neural network that was formed in block

1308 is satisfactory. If the performance is now found to be satisfactory then the process 1300 halts. If on the other hand it is found that the performance is still not satisfactory, then the process 1300 continues with block 1314 in which it is determined if a prescribed node limit has been reached. The node limit is preferably a value set by the user. If it is determined that the node limit has been reached then the process 1300 halts. If on the other hand the node limit has not been reached then the process 1300 loops back to block 1308 in which the number of nodes is again incremented and the thereafter the process continues as described above until either satisfactory performance is attained or the node limit is reached.

[Para 140] If in block 1306 it is determined that the performance of the neural network is satisfactory, then in order to try to reduce the complexity of the neural network, the process 1300 continues with block 1316 in which the number of processing nodes of the neural network is decreased. As before, the type of topology shown in FIG. 1 is preferably maintained when reducing the number of processing nodes. Next in block 1318 the neural network formed in the preceding block 1316 by decrementing the number of nodes is trained until the aforementioned stopping condition is met. Next, in block 1320 it is determined if the performance of the network trained in block 1318 is satisfactory. If it is determined that the performance is satisfactory then the process 1300 loops back to block 1316 in which the number of nodes is again decremented and thereafter the process 1300 proceeds as described above. If on the other hand it is determined that the performance is not satisfactory, then the parameters (e.g., number of nodes, weights) of the last satisfactory neural network are saved in block 1322 and the process halts. Rather than halting, as described above, other blocks are alternatively added to the processes shown in FIG. 7 and FIG. 13.

[Para 141] By utilizing the process 1300 for finding the minimum number of nodes required to achieve a predetermined accuracy in combination with an objective function that includes a term intended to reduce the number of weights of significant magnitude, reduced complexity neural networks can be

realized. Such reduce complexity neural networks can be implemented using less die space, dissipate less power, and are less prone to over-training.

[Para 142] The neural networks having sizes determined by process 1300 are implemented in software or hardware.

[Para 143] The processes depicted in FIGs. 7,13 are preferably embodied in the form of one or more programs that can be stored on a computer-readable medium which can be used to load the programs into a computer for execution. Programs embodying the invention or portions thereof may be stored on a variety of types of computer readable media including optical disks, hard disk drives, tapes, programmable read only memory chips. Network circuits may also serve temporarily as computer readable media from which programs taught by the present invention are read.

[Para 144] FIG. 14 is a block diagram of a computer 1400 used to execute the algorithms shown in FIGs. 7, 13 according to the preferred embodiment of the invention. The computer 1400 comprises a microprocessor 1402, Random Access Memory (RAM) 1404, Read Only Memory (ROM) 1406, hard disk drive 1408, display adopter 1410, e.g., a video card, a removable computer readable medium reader 1414, a network adapter 1416, keyboard 1418, and I/O port 1420 communicatively coupled through a digital signal bus 1426. A video monitor 1412 is electrically coupled to the display adapter 1410 for receiving a video signal. A pointing device 1422, preferably a mouse, is electrically coupled to the I/O port 1420 for receiving electrical signals generated by user operation of the pointing device 1422. According to one embodiment of the invention, the network adapter 1416 is used, to communicatively couple the computer to an external source of training data, and/or programs embodying methods 700, 1300 such as a remote server. The computer readable medium reader 1414 preferably comprises a Compact Disk (CD) drive. A computer readable medium 1424 that includes software embodying the algorithms described above with reference to FIGs. 7,13 is provided. The software included on the computer readable medium is loaded through the removable computer readable medium reader 1414 in order to configure the computer 1400 to carry out processes of the current invention that are described above

with reference to flow diagrams. The computer 1400 may for example comprise a personal computer or a workstation computer.

[Para 145] While the preferred and other embodiments of the invention have been illustrated and described, it will be clear that the invention is not so limited. Numerous modifications, changes, variations, substitutions, and equivalents will occur to those of ordinary skill in the art without departing from the spirit and scope of the present invention as defined by the following claims.